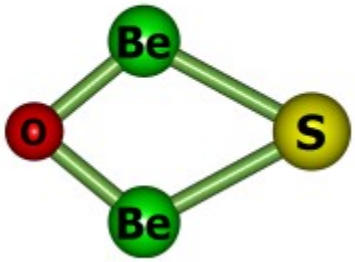
Supporting Information

of

Comment on "Strong Be–Be bonds in double-aromatic bridged Be2(μ-SO) molecules" by F. Rezaie and S. Noorizadeh, Dalton Transactions, 2022, 51, 12596

Cartesian coordinates of the optimized geometries along with their total energies (a.u) calculated at ωB97XD/cc-pVTZ.

$(C_{2V}, {}^1A_1)$



Sum of electronic and zero-point Energies= -503.047009

Sum of electronic and thermal Energies= -503.043446

Sum of electronic and thermal Enthalpies= -503.042502

Sum of electronic and thermal Free Energies= -503.072943

4	0.577172000	-0.923579000	-0.001523000
4	0.576997000	0.923811000	-0.001522000
8	1.699587000	-0.000041000	0.000920000
16	-1.138336000	-0.000037000	0.000301000

$(C_{\infty V}, {}^3A_1)$

Sum of electronic and zero-point Energies= -502.994900

Sum of electronic and thermal Energies= -502.989900

Sum of electronic and thermal Enthalpies= -502.988956

Sum of electronic and thermal Free Energies= -503.018848

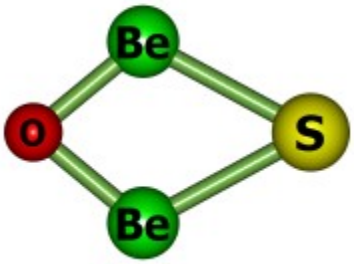
4	-3.077181000	-0.000101000	0.000015000

4 -0.257833000 0.003109000 -0.000004000

8 -1.667746000 -0.000825000 -0.000010000

16 1.667627000 -0.000339000 0.000002000

$(C_{2v}, {}^3A_1)$



Sum of electronic and zero-point Energies= -502.939685

Sum of electronic and thermal Energies= -502.935819

Sum of electronic and thermal Enthalpies= -502.934875

Sum of electronic and thermal Free Energies= -502.967113

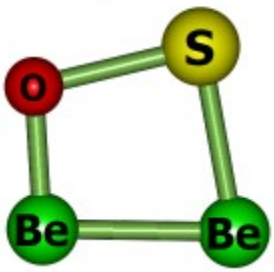
4 -0.636578000 -1.020895000 0.000023000

4 -0.637303000 1.021507000 0.000022000

8 -1.677774000 -0.000324000 -0.000117000

16 1.157357000 0.000009000 0.000047000

$(C_s, {}^1A')$



Sum of electronic and zero-point Energies= -502.882378

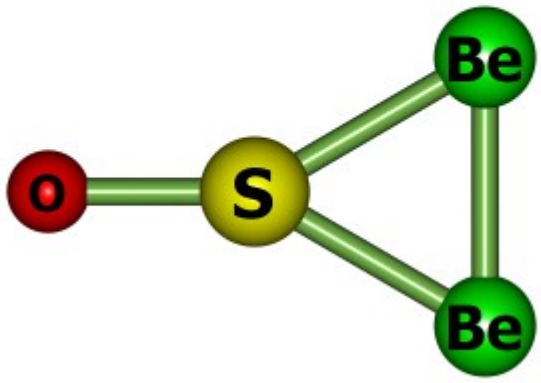
Sum of electronic and thermal Energies= -502.878100

Sum of electronic and thermal Enthalpies= -502.877156

Sum of electronic and thermal Free Energies= -502.909049

4	1.556015000	0.547425000	-0.000141000
4	-0.103090000	1.621739000	0.000105000
8	0.860863000	-0.727157000	0.000078000
16	-0.793663000	-0.178713000	-0.000030000

$(C_{2v}, {}^1A_1)$



Sum of electronic and zero-point Energies= -502.796226

Sum of electronic and thermal Energies= -502.791852

Sum of electronic and thermal Enthalpies= -502.790908

Sum of electronic and thermal Free Energies= -502.822939

4	-1.626189000	0.972744000	0.000132000
4	-1.627293000	-0.971795000	0.000134000
8	1.540415000	0.000171000	0.000089000
16	0.043163000	-0.000323000	-0.000111000